

Dibenzodioxin, 1,2,6,9-tetrabromo-, 3,7-dichloro-

Other names:	1,2,6,9-tetrabromo-3,7-dichloro-dibenzo-p-dioxin
Inchi:	InChI=1S/C12H2Br4Cl2O2/c13-3-1-4(17)8(15)12-10(3)20-11-6(19-12)2-5(18)7(14)9(11)1
InchiKey:	ABJGDNKUQDETRQ-UHFFFAOYSA-N
Formula:	C12H2Br4Cl2O2
SMILES:	Clc1cc2c(c(Br)c1Br)Oc1c(Br)cc(Cl)c(Br)c1O2
Mol. weight [g/mol]:	568.66

Physical Properties

Property code	Value	Unit	Source
gf	139.68	kJ/mol	Joback Method
hf	-0.57	kJ/mol	Joback Method
hfus	56.46	kJ/mol	Joback Method
hvap	95.73	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	7.941		Crippen Method
mcvol	227.780	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook
tb	967.70	K	Joback Method
tc	1266.25	K	Joback Method
tf	755.88	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.76	J/molxK	967.70	Joback Method
cpg	442.66	J/molxK	1017.46	Joback Method
cpg	449.93	J/molxK	1067.22	Joback Method
cpg	457.76	J/molxK	1116.97	Joback Method
cpg	466.35	J/molxK	1166.73	Joback Method
cpg	475.92	J/molxK	1216.49	Joback Method

cpg	486.67	J/mol×K	1266.25	Joback Method
dvisc	0.0005793	Paxs	755.88	Joback Method
dvisc	0.0004983	Paxs	791.18	Joback Method
dvisc	0.0004342	Paxs	826.49	Joback Method
dvisc	0.0003826	Paxs	861.79	Joback Method
dvisc	0.0003405	Paxs	897.09	Joback Method
dvisc	0.0003058	Paxs	932.40	Joback Method
dvisc	0.0002767	Paxs	967.70	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R170853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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